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EXPLICIT DIFFERENCE SCHEMES FOR WAVE PROPAGATION AND IMPACT PROBLEMS*

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ABSTRACT. Explicit finite difference and finite element schemes are constructed to solve wave propagation, shock, and impact problems. The schemes rely on exponential functions and the solution of linearized Riemann problems in order to reduce the effects of numerical dispersion and diffusion. The relationship of the new schemes to existing explicit schemes is analyzed and numerical results and comparisons are presented for several examples.

I. INTRODUCTION. Exponentially fitted and/or weighted finite difference [9,11], finite element [3,9,10], and collocation [5] schemes have become popular and effective methods of solving steady convection-diffusion problems. They avoid the spurious mesh oscillations that are found near boundary and shock layers when centered schemes are used at high cell Reynolds or Peclet numbers and they reduce the effects of numerical diffusion that are associated with classical upwind difference schemes.

We seek to extend exponential methods to transient problems and as a first step we consider one-dimensional scalar initial value problems of the form

$$u_t + f(u)_x = \varepsilon u_{xx} \quad , \quad t > 0 \quad , \quad |x| < \infty$$

$$u(x,0) = u^0(x) \quad , \quad |x| < \infty \qquad (1)$$

where $0 < \varepsilon \ll 1$ is either a real or an artificial viscosity parameter and the x and t subscripts denote partial differentiation.

Our primary motivation for studying exponential schemes is a desire to develop improved numerical methods for elastic-plastic impact problems in solids and blast problems in gases.

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In this paper, we confine our attention to explicit difference approximations of (1) having the form

$$U^{n+1}_j = U^n_j - \frac{1}{2}\lambda[(1 + z^n_{j-1/2})(f^n_j - f^n_{j-1}) + (1 - z^n_{j+1/2})(f^n_{j+1} - f^n_j)]$$

$$+ \frac{\varepsilon\lambda}{\Delta x}(U^n_{j-1} - 2U^n_j + U^n_{j+1}) \quad , \quad n > 0 \quad , \quad |j| < \infty$$

$$U^0_j = u^0(j\Delta x) \quad , \quad |j| < \infty \tag{2}$$

where Δx and Δt denote the uniform spatial and temporal grid spacings, respectively, U^n_j is the numerical approximation of $u(j\Delta x, n\Delta t)$,

$$f^n_j := f(U^n_j) \quad , \quad \lambda = \Delta t/\Delta x \tag{3,4}$$

and $z^n_{j+1/2}$ are upwind weighting factors.

Many popular difference schemes have the form of (2) and some of these are discussed and compared in Section II. We also introduce an exponential scheme that is based on determining $z^n_{j\pm1/2}$ so that U^n_j is the exact solution of the linearized steady equation

$$cu_x = \varepsilon u_{xx} \tag{5}$$

when $c = f'(u)$ is a constant. We call this method the linearized steady exponential (LSE) method and it is the simplest extension of the exponentially fitted and weighted schemes [3,9,10,11] to transient problems. The scheme gives improved accuracy for steady shock problems, but offers little improvement over classical upwind differencing for moving shock problems.

In Section III we develop an exponential scheme that is based on the exact solution of a linearized transient equation (1) that is subject to piecewise constant initial data, i.e., a linearized Riemann problem for (1). We call this method the linearized transient exponential (LTE) method and, like other methods based on the solutions of Riemann problems [1,2,4,6,8,13, 15,16], it sharply resolves boundary and shock layers without added diffusion or spurious oscillations. As $\varepsilon \to 0$ the LTE method becomes formally equivalent to Roe's method [15,16] for hyperbolic systems of conservation laws. van Leer [17] has noted that Roe's method treats an expansion fan as a so called "expansion shock" (cf. Figure 6) and, unfortunately, our LTE method also has this disturbing property even when ε is nonzero, but small.

In Section IV we present some preliminary results for vector systems of equations and in Section V we discuss our results and indicate some directions for future work.

II. THE LINEARIZED STEADY EXPONENTIAL (LSE) METHOD. The LSE method is obtained from (2) by selecting z^n_k, $k = j\pm1/2$, as

$$z^n_k = \coth \rho^n_k/2 - 2/\rho^n_k \tag{6}$$

where ρ^n_k is the cell Reynolds number

$$\rho^n_k = \frac{\Delta x}{\varepsilon}\left(\frac{c^n_{k+1/2} + c^n_{k-1/2}}{2}\right) \tag{7}$$

and

$$c^n_j := f'(U^n_j) \tag{8}$$

As previously noted, the LSE method will give a pointwise exact steady state solution of (1) when c^n_j is a constant. This or similar schemes have been used by several investigators [3,9,10,11] for steady singularly-perturbed problems and herein we try to apply it to transient problems.

We first consider a linear stability analysis of the difference scheme (2) by letting $f(u) = cu$ where c is a constant. We also let ρ and z denote the constant values of ρ^n_k and z^n_k, respectively, α denote the Courant number

$$\alpha = c\Delta t/\Delta x \tag{9}$$

and β denote the dissipation parameter

$$\beta = \alpha(z + 2/\rho) \tag{10}$$

In this case, equation (2) can be written as

$$U^{n+1}_j = U^n_j - \frac{1}{2}\alpha(U^n_{j+1} - U^n_{j-1}) + \frac{1}{2}\beta(U^n_{j+1} - 2U^n_j + U^n_{j-1}) \tag{11}$$

Several popular difference schemes have the form of (11) for different values of β (or z) and some of these are listed in Table 1. All of these schemes are first order accurate in time, except the Lax-Wendroff scheme which is second order.

A von Neumann analysis (cf. Richtmyer and Morton [14]) shows that equation (11) is stable in the region $\alpha^2 < \beta$, $0 < \beta < 1$. This region is shown shaded for $\alpha > 0$ in Figure 1. Curves corresponding to the methods in Table 1 are also shown. We see that the LSE method slightly improves upon the stability and accuracy properties of upwind differencing and that centered differencing and the Lax-Friedrichs scheme are outside of the stability region for most values of α and β.

<u>Example 1</u>: We compare the methods in Table 1 on the constant coefficient initial-boundary value problem

$$u_t + u_x = \varepsilon u_{xx}\ , \quad t > 0\ , \quad 0 < x < 1$$

$$u(x,0) = 0\ , \quad 0 < x < 1$$

$$u(0,t) = 1\ , \quad u(1,t) = 0 \tag{12}$$

The exact solution of this problem features a shock layer that moves from x = 0 to x = 1 with unit speed and then approaches the steady state solution

$$u(x,t) = \frac{1 - e^{-(1-x)/\varepsilon}}{1 - e^{-1/\varepsilon}} \qquad (13)$$

as $t \to \infty$.

The maximum error at steady state

$$\max_j |u(j\Delta x, n\Delta t) - U^n_j| \quad , \quad n \to \infty \qquad (14)$$

computed by the Lax-Wendroff, upwind, LSE, and Lax-Friedrichs schemes are shown in Table 2 for $\Delta x = 1/20$, $\rho = 6$, $\alpha = 0.375, 0.75$ and $\Delta x = 1/20$, $\rho = 500$, $\alpha = 0.475, 0.95$*.

The centered difference scheme produced overflows for both $\rho = 6$ and 500, so no results could be listed for it. The Lax-Friedrichs scheme only overflowed for $\rho = 6$. The LSE scheme gives the exact steady state solution for this example and the small errors reported in Table 2 are due to the combined effects of roundoff and our failure to reach the exact steady state.

These results are very encouraging; however, when we examine the LSE solution during the transient phase of the solution the situation is quite different (cf. Figure 2). The LSE solution is overly diffusive and the computed solution is not much better than that obtained by upwind differencing. This observation was also noted by Gresho and Lee [7] about methods that are similar to the LSE method.

III. THE LINEARIZED TRANSIENT EXPONENTIAL (LTE) METHOD. We would like to improve upon the results of the LSE method for transient problems and, thus, we consider developing a method having the form of (2) that gives a pointwise exact solution of (1) when $f(u) = cu$ and c is a constant. Since we are primarily interested in obtaining good resolution near shock and boundary layers we choose to solve (1) subject to Riemann initial data. To be specific, for each j and n we compute U^{n+1}_j as the exact solution of the initial value problem.

$$u_t + cu_x = \varepsilon u_{xx} \quad , \quad t > n\Delta t \quad , \quad |x| < \infty \quad ,$$

$$u(x,n\Delta t) = \begin{cases} u_L \quad , & x < (j-1+\delta)\Delta x \\ u_R \quad , & x > (j-1+\delta)\Delta x \end{cases} \qquad (15)$$

where u_L and u_R are constants, δ is a constant on $[0,1)$ to be determined, and we assume that $c > 0$. We shall present results for $c < 0$ later.

The exact solution of (15) at $x = j\Delta x$ and $t = (n+1)\Delta t$ is

$$u(j\Delta x,n\Delta t) = u_R - \frac{1}{2}(u_R-u_L)\operatorname{erfc} \frac{1}{2}\sqrt{\frac{\rho}{\alpha}}(1-\delta-\alpha) \qquad (16)$$

*All numerical results were obtained in double precision on an IBM 4341 computer at the Benet Weapons Laboratory.

whereas the solution of equation (2) at this point is

$$U^{n+1}_j = u_R - \frac{1}{2}\alpha(1 + z^n_{j-1/2} + 2/\rho)(u_R-u_L) \tag{17}$$

The two solutions will be the same provided that

$$z^n_{j-1/2} = -1 - \frac{2}{\rho} + \frac{1}{\alpha}\,\mathrm{erfc}\,\frac{1}{2}\sqrt{\frac{\rho}{\alpha}}\,(1-\delta-\alpha) \tag{18}$$

In this paper, we simplify (18) by assuming that $\rho/\alpha >> 1$ and approximating the complementary error function by $2H(\delta+\alpha-1)$, where H is a Heaviside function. Also, since $z^n_{j+1/2}$ is not determined by this procedure, we specify it according to equation (6) with coth $\rho/2$ approximated by unity. Thus, we have

$$z^n_{j-1/2} = 1 - \frac{2}{\rho} + 2[\frac{1}{\alpha}H(\delta+\alpha-1) - 1] \quad , \quad z^n_{j+1/2} = 1 - \frac{2}{\rho} \tag{19a}$$

When $c < 0$ we choose

$$z^n_{j-1/2} = -1 - \frac{2}{\rho} \quad , \quad z^n_{j+1/2} = -1 - \frac{2}{\rho} + 2[\frac{1}{\alpha}H(\delta-\alpha-1) + 1] \tag{19b}$$

It remains to specify δ. One possibility is to choose it to be a random variable uniformly distributed on $[0,1)$, in which case equations (2) and (19) would yield a linearized random choice scheme [1,2]. A second possibility is to always select $\delta = 1/2$ which would give a Godunov [6] type scheme. The third possibility is similar to a scheme suggested by Roe [15] and is the one that we have been using. We begin by selecting $\delta = 0$; however, any value of $\delta\varepsilon[0,1)$ will do. After each time step we add the magnitude of the Courant number $|\alpha|$ to δ and obtain a new value of δ. We continue this process until δ exceeds unity, in which case we replace δ by $\delta-1$. The procedure has to be modified slightly when α is not a constant and we shall indicate how this is done shortly; however, if α is a rational number of the form p/q and $\varepsilon = 0$ then equations (2) and (19) have the advantage of giving the pointwise exact solution of the linearized Riemann problem every q time steps.

We refer to the scheme consisting of equations (2) and (19) and the above choice of δ as the linearized transient exponential (LTE) method and we begin by applying it to the following linear Riemann problem.

<u>Example 2</u>:

$$u_t + u_x = \varepsilon u_{xx} \quad , \quad t > 0 \quad , \quad |x| < \infty \tag{20}$$

$$u(x,0) = \begin{cases} 1 & , \quad x < 0 \\ 0 & , \quad x > 0 \end{cases}$$

In this example, the initial discontinuity becomes a shock layer which travels with unit speed in the positive x direction while widening as t increases.

We have computed the solution of this problem by the LTE method with $\Delta x = 1/20$, $\rho = 500$, and $\alpha = 0.75, 0.95$. For this value of ρ and for times less than order $1/\varepsilon$, the shock layer is well contained within one mesh subinterval

and we have plotted the locations of the ends of this subinterval along with the exact position of the center of the shock layer in Figures 3 and 4 for $\alpha = 0.75$ and 0.95, respectively. We see that the shock layer is tracked exactly on the average and that we obtain the pointwise exact solution every 4 and 20 time steps when $\alpha = 0.75$ and 0.95, respectively.

For nonlinear scalar problems we still use equations (2) and (19); however, we now use local values of the Courant and Reynolds numbers based on a local shock speed. Thus, on each subinterval we calculate

$$\alpha^n_{j-1/2} = s^n_{j-1/2}\Delta t/\Delta x \quad , \quad \rho^n_{j-1/2} = s^n_{j-1/2}\Delta x/\varepsilon \qquad (21a,b)$$

where $s^n_{j-1/2}$ is a local shock speed which we choose as

$$s^n_{j-1/2} = (f^n_j - f^n_{j-1})/(U^n_j - U^n_{j-1}) \qquad (22)$$

Equations (21) are used in equations (19) to calculate $z^n_{j-1/2}$ and we proceed as in the linear case. After each time step we add

$$(\min_j|\alpha^n_{j-1/2}| + \max_j|\alpha^n_{j-1/2}|)/2$$

to δ and obtain a new value of δ. Once δ exceeds unity we again replace it by $\delta-1$.

Equation (22) gives the exact shock speed whenever U^n_j and U^n_{j-1} satisfy the Rankine-Hugoniot jump conditions (cf. e.g. Whitham [18] and equation (27)). An alternate definition of $s^n_{j-1/2}$ that is easier to use computationally, but only gives the correct shock speed when f is at most a quadratic function of u is

$$s^n_{j-1/2} = \frac{1}{2}\,[f'(U^n_j) + f'(U^n_{j-1})] \quad . \qquad (23)$$

<u>Example 3</u>: We consider a Riemann problem for Burgers' equation

$$u_t + \frac{1}{2}(u^2)_x = \varepsilon u_{xx} \quad , \quad t > 0 \quad , \quad |x| < \infty \quad ,$$

$$u(x,0) = \begin{cases} u_L \quad , & x < 0 \\ u_R \quad , & x > 0 \end{cases} \qquad (24)$$

The exact solution of this problem can be obtained by the Hopf-Cole transformation and is given in, e.g., Whitham [18]. Herein, it suffices to give asymptotic formulas which are valid for $t/\varepsilon \gg 1$. Thus, when $u_L > u_R$ we have

$$u(x,t) \sim \frac{1}{2}(u_L + u_R) - \frac{1}{2}(u_L - u_R)\tanh\left(\frac{u_L - u_R}{4\varepsilon}\right)(x - St) \qquad (25a)$$

where

$$S = \frac{1}{2}(u_L + u_R) \qquad (25b)$$

and when $u_L < u_R$ we have

$$u(x,t) \sim \begin{cases} u_L \quad , & x/t < u_L \\ x/t \quad , & u_L < x/t < u_R \\ u_R \quad , & u_R < x/t \end{cases} \tag{26}$$

Equation (25) represents a shock layer moving in the positive x direction with speed S and equation (26) represents an expansion fan.

We calculated solutions with $\varepsilon = 10^{-4}$, $\Delta x = 1/20$, and $\lambda = 0.95$ by the LSE and LTE methods for a shock problem with $u_L = 1$, $u_R = 0$ and an expansion problem with $u_L = -1$, $u_R = -1/2$. In Figure 5 we compare the exact shock position with those calculated by the LSE and LTE methods. We define the shock position for the numerical methods as the point where the solution is $(u_L - u_R)/2$ when linear interpolation is used to compute solution values between mesh points. In Figures 6a and 6b we plot the exact LSE and LTE solutions at $t = 0.95$ for the shock problem and at $t = 0.38$ for the expansion problem, respectively. The LTE method again confines the shock layer to one subinterval and gives the correct shock speed and position on the average. The LSE method is overly diffusive and is giving the correct shock speed, but the position is wrong by about $\Delta x/2$.

The situation is quite different for the expansion fan. The LSE method is still overly diffusive; however, the LTE method is representing the expansion fan as a shock. This phenomenon also occurs with Roe's scheme for hyperbolic systems (cf. Roe [16] and van Leer [17]) and it must be remedied if these schemes are to be useful on expansion problems.

IV. SYSTEMS OF EQUATIONS. In principle the LTE method consisting of equation (2), (19), and (21) may be directly extended to vector systems of the form (1) once we have selected a shock speed $s^n_{j-1/2}$. When $\varepsilon = 0$ the exact shock speed S is determined by the Rankine-Hugoniot condition

$$(\underset{\sim}{u}_R - \underset{\sim}{u}_L)S = \underset{\sim}{f}(\underset{\sim}{u}_R) - \underset{\sim}{f}(\underset{\sim}{u}_L) \tag{27}$$

where $\underset{\sim}{u}_R$ and $\underset{\sim}{u}_L$ are the values of $\underset{\sim}{u}(x,t)$ on opposite sides of the shock. When ε is nonzero but small we would like the numerical shock speed $s^n_{j-1/2} = S$ whenever the numerical solution $\underset{\sim}{U}^n_{j-1}$, $\underset{\sim}{U}^n_j$ satisfies (29).

In a recent paper Harten and Lax [8] suggested selecting

$$s^n_{j-1/2} = \ell(\underset{\sim}{f}^n_j - \underset{\sim}{f}^n_{j-1})/\ell(\underset{\sim}{U}^n_j - \underset{\sim}{U}^n_{j-1}) \tag{28a}$$

where $\ell(\underset{\sim}{w})$ is the linear functional

$$\ell(\underset{\sim}{w}) = [V'(\underset{\sim}{U}^n_j) - V'(\underset{\sim}{U}^n_{j-1})]\underset{\sim}{w} \tag{28b}$$

and $V(\underset{\sim}{u})$ is an entropy function. They show that this choice gives unique physically admissible numerical solutions of their random choice finite difference methods.

Roe [16] suggests an alternate method of calculating $s^n_{j-1/2}$ that is based on the eigenvalue of a matrix approximating the Jacobian $\partial \underset{\sim}{f}/\partial \underset{\sim}{u}$.

We have not tried either of these alternatives, but instead use the very simple prescription

$$s^n_{j-1/2} = \frac{(\underset{\sim}{U}^n_j - \underset{\sim}{U}^n_{j-1})^T(\underset{\sim}{f}^n_j - \underset{\sim}{f}^n_{j-1})}{(\underset{\sim}{U}^n_j - \underset{\sim}{U}^n_{j-1})^T(\underset{\sim}{U}^n_j - \underset{\sim}{U}^n_{j-1})} \qquad (29)$$

Equation (29) gives the exact shock speed whenever U^n_j and U^n_{j-1} satisfy the Rankine-Hugoniot conditions (27), but it may fail to give a physically acceptable solution.

Example 4: We solve the following impact problem for the linear wave equation

$$u_{1t} - u_{2x} = 0 \quad , \quad u_{2t} - u_{1x} = 0 \quad , \quad t > 0 \quad , \quad |x| < \infty$$

$$u_1(x,0) = 0 \quad , \quad u_2(x,0) = \begin{cases} 1 \quad , & x < 0 \\ -1 \quad , & x > 0 \end{cases} \qquad (30)$$

Here $u_1(x,t)$ and $u_2(x,t)$ represent the strain and velocity in two elastic rods that impact each other with unit speeds at $x = t = 0$.

We calculated the solution of this problem by the LSE and LTE methods and by the EPIC-2 code [12]. The latter is a two-dimensional finite element code for elastic-plastic impact problems. Our results for u_1 at $t = 0.95$ obtained with $\Delta x = 1/10$ and $\lambda = 0.95$ are shown in Figure 7. The LSE and LTE solutions are typical of our results on previous examples. The LTE method again calculates the correct shock position and speed with no diffusion or oscillations. The LSE solution is overly diffusive, although less so than the EPIC-2 solution.

V. DISCUSSION OF RESULTS. The LTE method appears to be a very promising scheme for shock problems. It is simpler to apply than methods based on the exact solution of Riemann problems [1,2] and does not suffer from the effects of artificial diffusion or spurious oscillations. However, our results are very preliminary and there are still many questions to be answered and many problems to be overcome. The performance of the LTE method in regions of expansion must be improved. van Leer [17] has suggested incorporating expansion fans in the approximate Riemann solution of Roe's method [16], and this approach should work for our LTE method as well. Another possibility is to base the difference scheme (2) on the exact solution of (1) when f is a quadratic function of u. The solution of this problem does contain expansion waves; however, extending this method to systems of equations would be considerably more difficult than extending the LTE method.

Both the LSE and LTE methods are first order accurate in time when the solution is smooth. van Leer [17] has developed a two-step procedure that can be used to extend these methods to second order accuracy and we plan to experiment with it shortly.

There is also the possibility of developing implicit exponentially fitted and weighted schemes, which would be desirable when approaching a steady state and which may improve the phase characteristics of the LSE method (cf. Gresho and Lee [7]).

Finally, we note that the LSE and LTE methods can be extended to higher dimensions by using operator splitting techniques. However, this may introduce some numerical diffusion.

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TABLE 1. VALUES OF z AND β FOR DIFFERENCE METHODS THAT HAVE THE FORM OF EQUATION (11)

Method	z	$\beta = \alpha(z + 2/\rho)$
Centered	0	$2\alpha/\rho$
Lax-Wendroff	α	$\alpha^2 + 2\alpha/\rho$
Upwind	$\mathrm{sgn}(\rho)$	$\alpha(\mathrm{sgn}(\rho) + 2/\rho)$
Linearized steady exponential (LSE)	$\coth(\rho/2) - 2/\rho$	$\alpha\coth(\rho/2)$
Lax-Friedrichs	$1/\alpha$	$1 + 2\alpha/\rho$

TABLE 2. MAXIMUM ERROR AT STEADY STATE FOR EXAMPLE 1. AN * INDICATES THAT THE COMPUTED SOLUTION PRODUCED AN OVERFLOW.

Method	$\rho = 6$		$\rho = 500$	
	$\alpha = 0.375$	0.75	$\alpha = 0.475$	0.95
Lax-Wendroff	2.9 E-1	1.6 E-3	3.5 E-1	2.3 E-2
Upwind	2.0 E-2	2.0 E-2	2.0 E-3	2.0 E-3
Linearized steady exponential (LSE)	2.5 E-14	2.5 E-14	8.5 E-8	2.1 E-12
Lax-Friedrichs	*	*	3.6 E-1	2.8 E-2

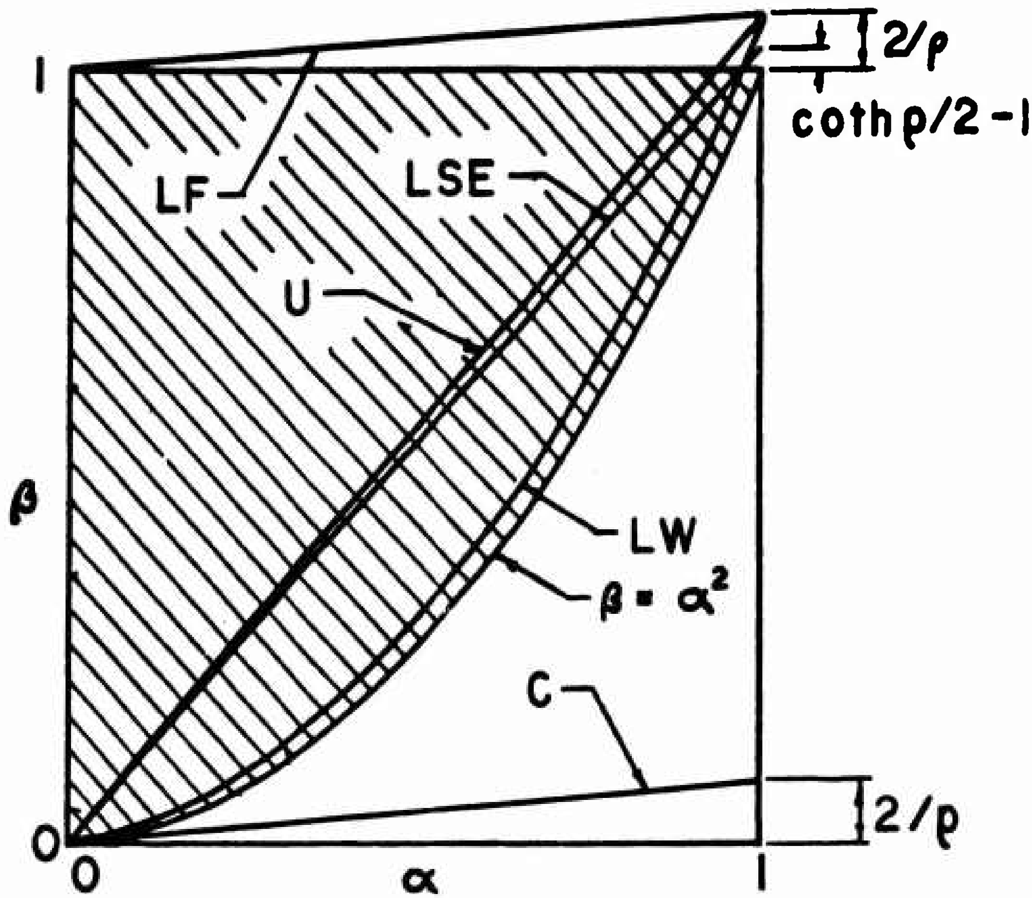

Figure 1. Region of linear stability for equation (11) and curves of β vs. α for the centered difference (C), Lax-Wendroff (LW), upwind difference (U), linearized steady exponential (LSE), and Lax-Friedrichs (LF) methods.

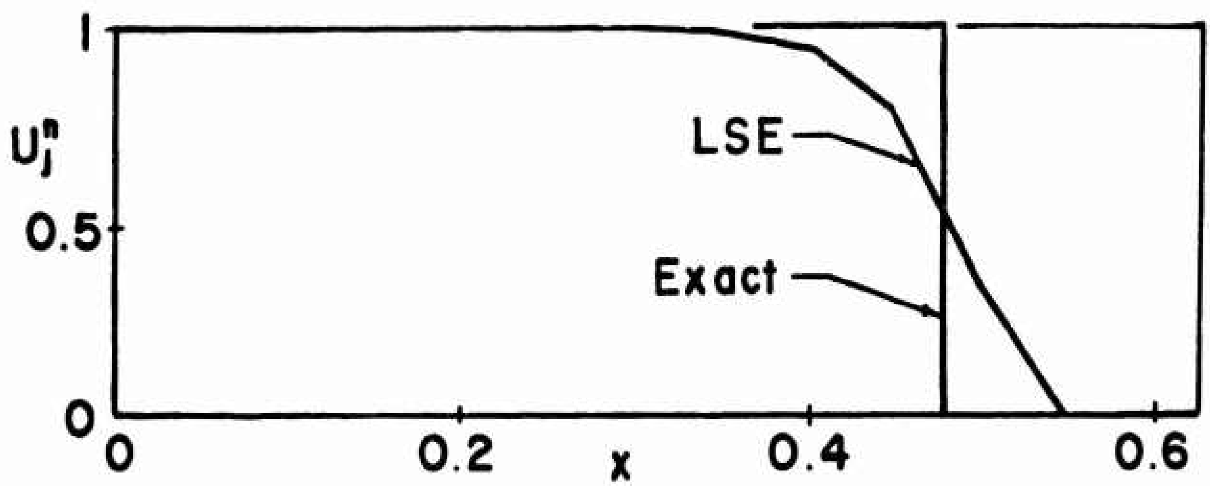

Figure 2. Comparison of exact and LSE solutions of Example 1 at $t = 0.475$. Calculations were performed with $\Delta x = 1/20$, $\alpha = 0.95$, and $\rho = 500$.

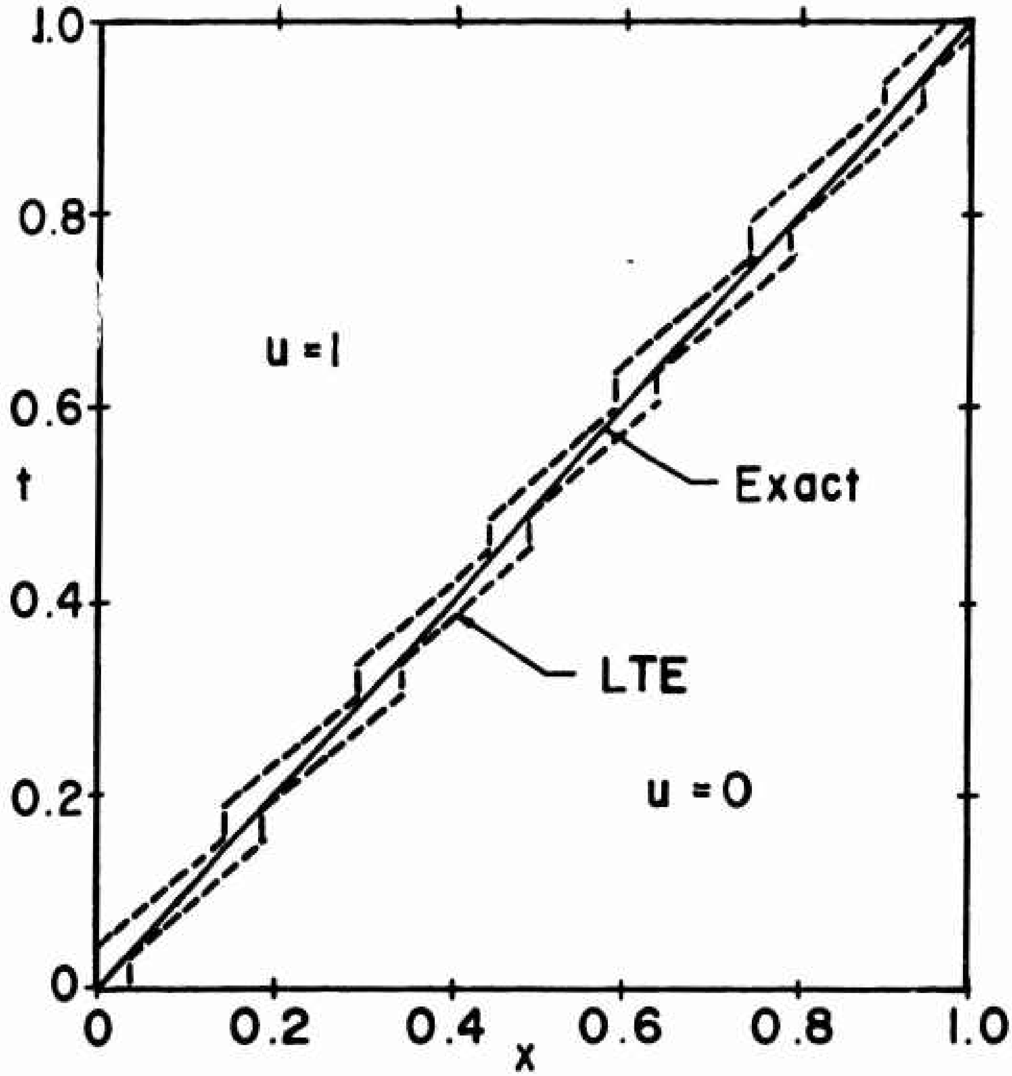

Figure 3. Exact shock layer position and the location of the subinterval containing the shock layer calculated by the LTE method for Example 2 with $\Delta x = 1/20$, $\alpha = 0.75$, and $\rho = 500$.

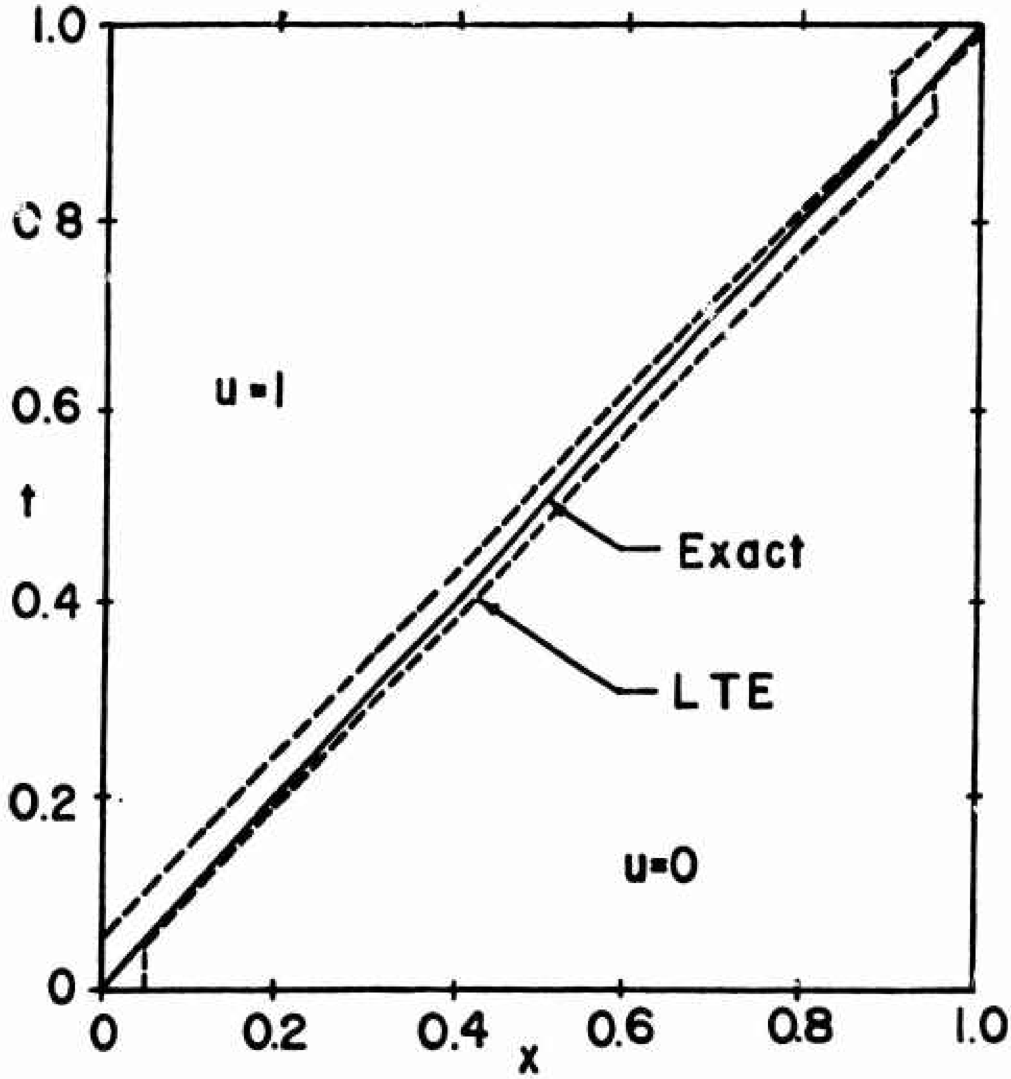

Figure 4. Exact shock layer position and the location of the subinterval containing the shock layer calculated by the LTE method for Example 2 with $\Delta x = 1/20$, $\alpha = 0.95$, and $\rho = 500$.

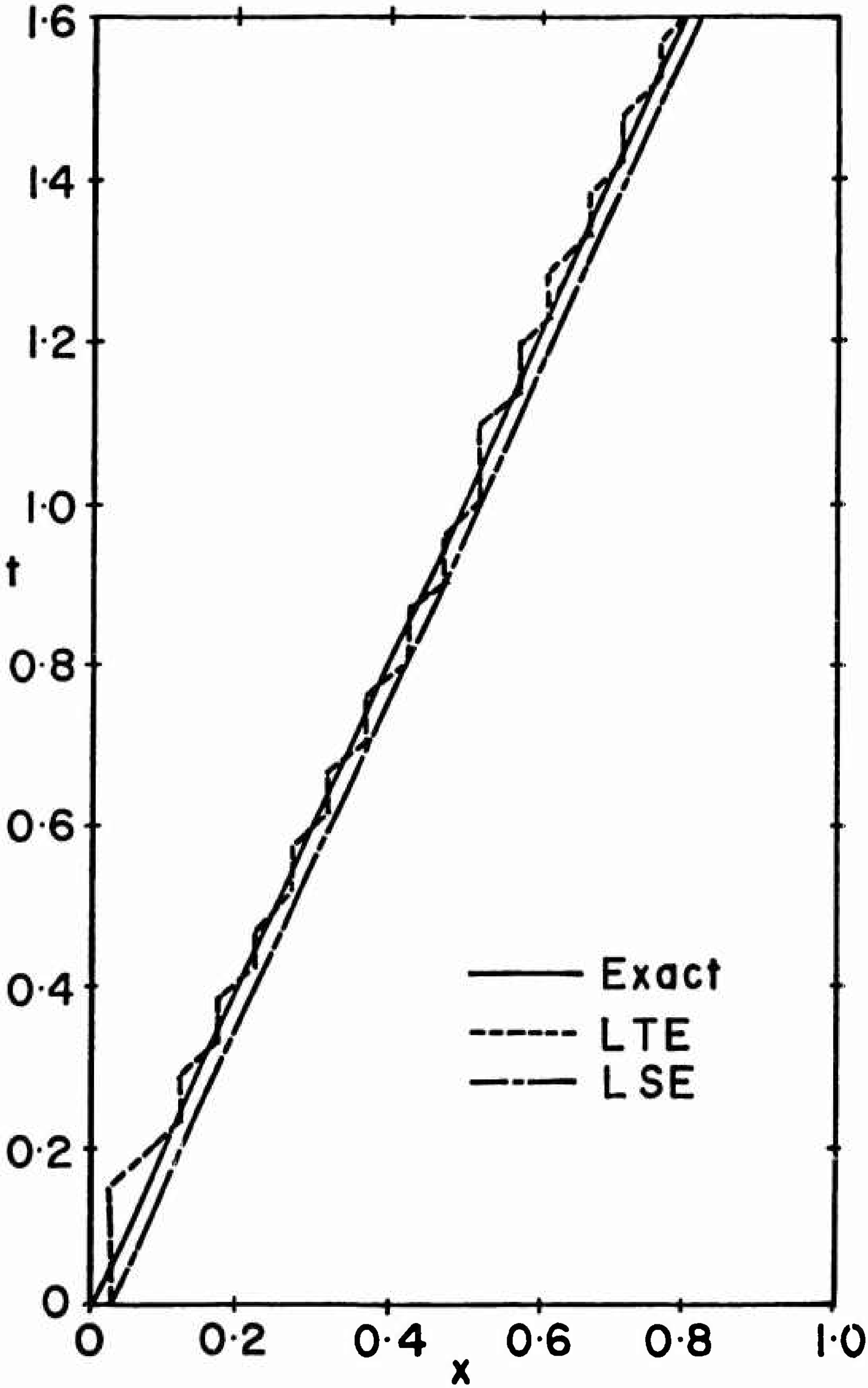

Figure 5. Exact shock layer position and those calculated by the LSE and LTE methods for Example 3 with $\varepsilon = 10^{-4}$, $\Delta x = 1/20$, and $\alpha = 0.95$.

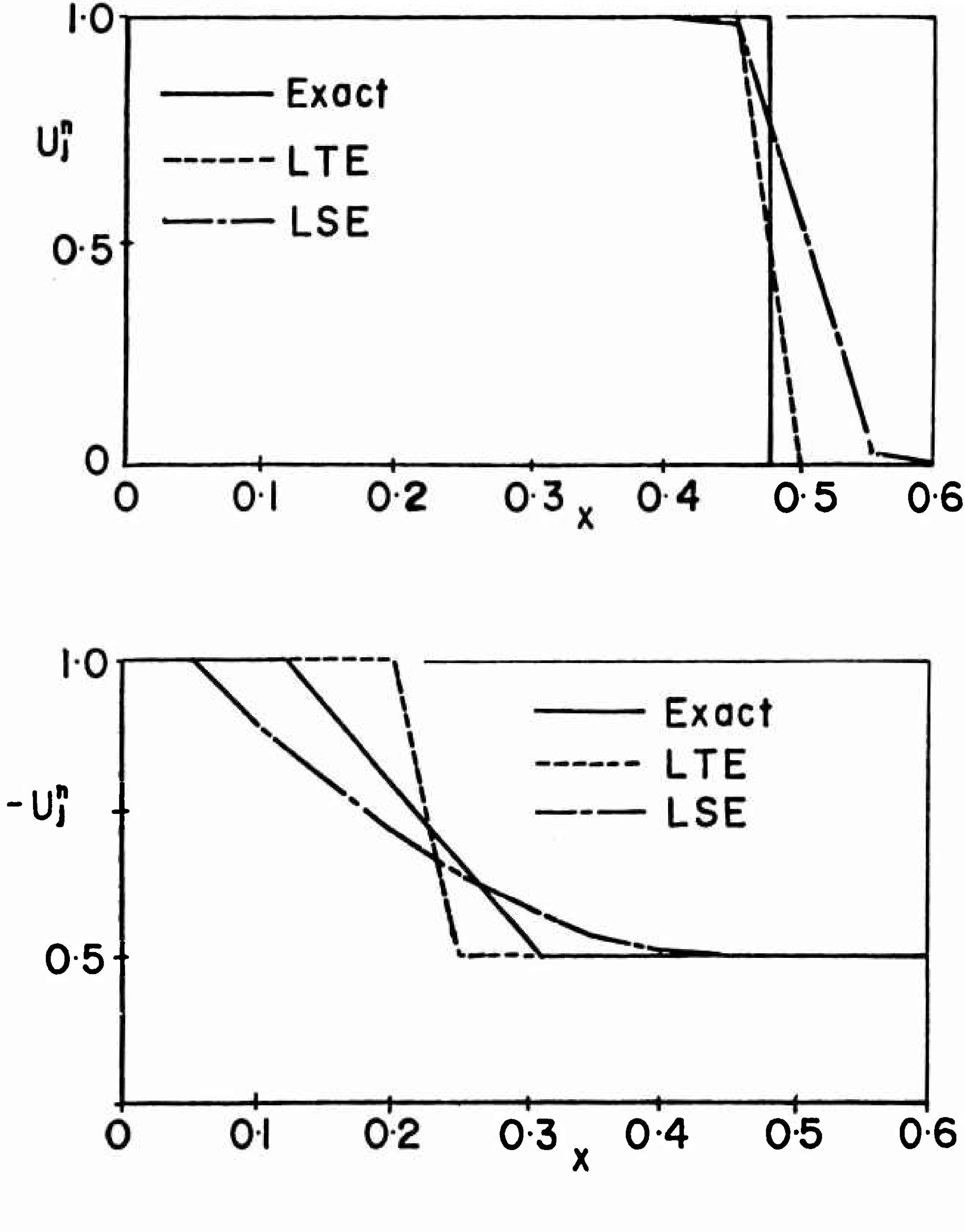

Figure 6. Exact, LSE, and LTE solutions of Example 3 with $\varepsilon = 10^{-4}$, $\Delta x = 1/20$, and $\alpha = 0.95$. In (a) we show the solution at $t = 0.95$ of a shock problem with $u_L = 1$, $u_R = 0$, and in (b) we show the solution at $t = 0.38$ of an expansion problem with $u_L = -1$, $u_R = -1/2$.

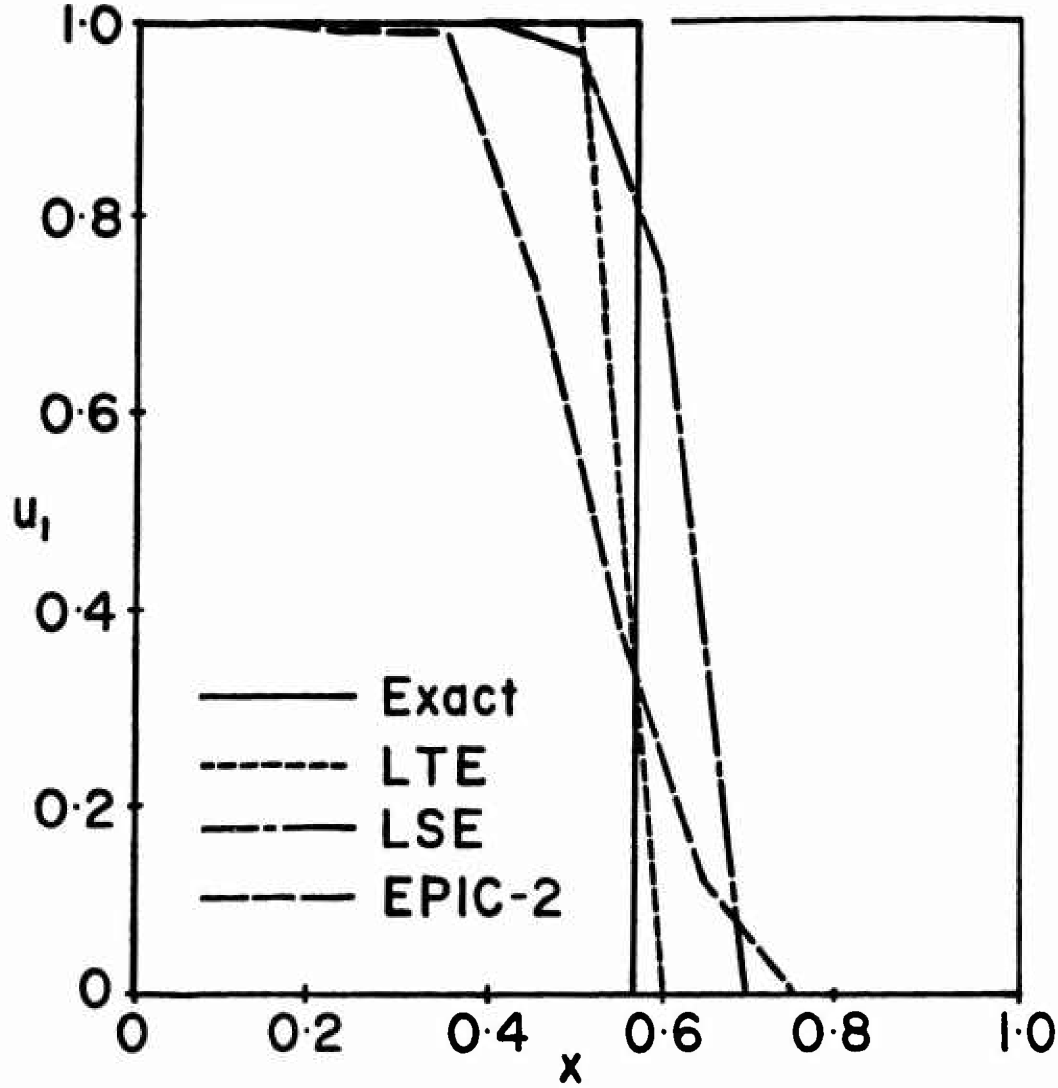

Figure 7. Comparison of exact, LSE, LTE, and EPIC-2 solutions for u_1 of Example 4 at $t = 0.95$ with $\Delta x = 0.1$ and $\Delta t = 0.095$.